

201-14744



Aromatic Sulfonic Acids Association

1850 M Street, NW, Suite 700, Washington, DC 20036
(202) 721-4100 – (202) 296-8120 fax

September 16, 2003

The Honorable Marianne Horinko, Acting Administrator
U.S. Environmental Protection Agency
P.O. Box 1473
Merrifield, VA 22116

RECEIVED
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Re: Aromatic Sulfonic Acids Association (ASAA) Submission of HPV Test Plan and Robust Summaries under the Chemical Right-to-Know Program for hydroxybenzene sulfonic acid (CAS No. 1333-39-7)

Dear Administrator Horinko:

The Aromatic Sulfonic Acids Association submits the attached test plan for hydroxybenzene sulfonic acid (CAS No. 1333-39-7) including robust summaries in IUCLID format under the High Production Volume Chemicals Challenge Program.

Please direct any comments to the ASAA Executive Director, William Smock at William.Smock@verizon.net.

Sincerely,

William H. Smock
Executive Director

201-14744A

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**HPV Assessment Report
On
Hydroxybenzenesulphonic acid
CAS No. 1333-39-7**

September 12, 2003

**Submitted on behalf of the Aromatic Sulfonic Acids Association
1850 M Street, NW, Suite 700, Washington DC 20036**

**Prepared by NOTOX Safety and Environmental Research B.V.
for submission under the US-HPV Challenge Program**

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1. Introduction

Capital Resin Corporation, Dynachem, Inc. and Rutgers Organics Corporation formed a consortium known as the Aromatics Sulfonic Acids Association (ASAA) to participate in the United States High Production Volume (HPV) Challenge Program for hydroxybenzenesulphonic acid, (CAS 1333-39-7). Hydroxybenzenesulphonic acid is one of several sulphonic acid based industrial chemicals used as a chemical intermediate and a resin binding catalyst. The substance is classified as a high production volume (HPV) chemical according to criteria established by the US-EPA, (i.e., > 1,000,000 pounds manufactured or imported into the USA annually). The consortium has agreed to provide all internal documents related to the requirements of the Challenge Program and/or initiate scientifically justified studies for this chemical substance as required to meet the needs of the HPV Chemical Challenge Program.

Under agreement with the consortium, NOTOX Safety and Environmental Research B.V. has conducted an evaluation and assessment of the available data on hydroxybenzenesulphonic acid (CAS 1333-39-7). No data were available from sponsors. For the development of screening health and environmental assessment information, NOTOX examined the public literature. A literature search performed in March 2003 did not yield any additional results to the existing data in the ECB IUCLID. Then the suitability of studies retrieved on hydroxybenzenesulphonic acid for meeting the SIDS data requirements was determined (summarised in chapter 2), a SIDS data matrix was constructed and recommendations for the draft testing scheme were formulated (data availability analysis; chapter 3). Robust summaries are presented in separate documents as IUCLID data sets.

2. Evaluation of SIDS endpoints

In this chapter an evaluation of data available on SIDS endpoints is given.

The substance under consideration is a sulphonic acid. Hydroxybenzenesulphonic acid is very acidic and in watery environments it is almost completely ionised, even at low pH. The substance is sold as a commercial preparation of 60-70% in water and contains less than 2% phenol and less than 3% sulphuric acid.

2.1. Physico-chemical endpoints

Adequate data on melting point, boiling point, relative density and vapour pressure all are available. The measured value for water solubility is confirmed by the calculated value. The partition coefficient was calculated to be very low as expected from the structural formula; the substance dissolves to a much larger extent in water than in octanol. The dissociation constant for the sulphonic acid group as well as for the hydroxyl group were calculated to be -2.19 and 9.05. This means that the sulphonic acid will be primarily ionised in water.

Conclusion: For the physico-chemical endpoints all relevant endpoints are sufficiently investigated.

Hydroxybenzenesulphonic acid CAS 1333-39-7				
	Value	Comment	KL	Ref
Melting point (°C)	129	calculated	2	3
Boiling point (°C)	270	MSDS	4	1,2
Relative Density	1.35	MSDS	4	1,2
Vapor pressure (hPa)	4.4E-07	calculated	2	3
Partition coefficient (log K _{ow})	-1.65	calculated	2	3
Water solubility (g/L)	100 vol%		4	1,2
	1000	calculated	2	3
Dissociation constant (pKa)	-2.19/9.05	calculated	2	4

KL = Klimisch criteria

Ref = Reference number

2.2. Environmental fate

The half-life for reaction of hydroxybenzenesulphonic acid with hydroxyl radicals in the atmosphere was estimated to be 17.3 hours. No hydrolysable groups are present in hydroxybenzenesulphonic acid. Distribution in the environment was calculated at Mackay Level III. If the sulphonic acid is released to the environment it will be to the water compartment and stay there (see table below)..

For biodegradability no data are available. From non-standard tests available on p-hydroxybenzenesulphonic acid (one of the components of hydroxybenzenesulphonic acid) it seems likely that hydroxybenzenesulphonic acid is not readily biodegradable. This is confirmed by the calculated probability for MITI linear biodegradation by EPISuite (0.3 = not readily biodegradable). To confirm that hydroxybenzenesulphonic acid is biodegradable an inherently biodegradability test is recommended.

Conclusion: For all relevant endpoints on environmental fate, data are available, except for biodegradation. Therefore, a biodegradation study testing inherent biodegradation has to be

performed.

Hydroxybenzenesulphonic acid CAS 1333-39-7				
	Value	Comment	KL	Ref
Photodegradation (t1/2)	17.3 hours		2	3
Hydrolysis (t1/2)	-			
Distribution in water/air/soil/sediment	99.8/0. /0.0/0.17%	calculated (emission to water only)	2	3
Biodegradability	-			

KL = Klimisch criteria

Ref = Reference number

2.3. Ecotoxicity

For ecotoxicity no measured data are available. Calculation of the relevant endpoints with the ECOSAR model predicts that hydroxybenzenesulphonic acid is not toxic for aquatic species.

Conclusion: Two of the species should be tested. If the resulting measured data are in agreement with the calculated data no further testing is warranted; if the resulting measured data disagree with the calculated data also the third species has to be tested.

Hydroxybenzenesulphonic acid CAS 1333-39-7				
	Value	Comment	KL	Ref
Acute fish (96-h LC50, mg/L)	45329	calculated	4	3
Acute invertebrates (48-h EC50, mg/L)	2916	calculated	4	3
Algal inhibition (96-h EC50, mg/L)	1.5E06	calculated	4	3

KL = Klimisch criteria

Ref = Reference number

2.4. Mammalian toxicity

2.4.1. Acute toxicity

Two oral route values for rat and mouse are available of 1900 and 1500 mg/kg bw, respectively. Since these values are similar, no further testing is considered necessary.

2.4.2. Genetic toxicity

No data are available, so an Ames test and a chromosomal aberration study are warranted.

2.4.3. Repeated dose toxicity

No data are available, so repeated dose toxicity can be considered a data gap. A 28-day repeated dose study must be performed.

2.4.4. Repro/developmental toxicity

No data are available on this endpoint, so a repro/developmental study should be performed.

Conclusion mammalian toxicity: Acute toxicity has been sufficiently investigated. For genetic toxicity an Ames test and a chromosomal aberration test need to be performed. Repeated dose toxicity needs to be covered with a 28-day study. Repro/developmental toxicity needs to be investigated. Based on the data available this can most appropriately be executed in a combined study with repeated dose toxicity (OECD422).

Hydroxybenzenesulphonic acid CAS 1333-39-7				
	Value	Species	KL	Ref
Acute toxicity				
Acute oral (LD50, mg/kg)	1900	rat	4	8, 9
	1500	mouse	4	
Acute dermal (LD50, mg/kg)	-			
Acute inhalation (LC50, mg/m ³)	-			
Genetic toxicity				
in vitro gene mutation (Ames test)	-			
Chromosomal aberration	-			
Repeated dose	-			
Repro/developmental toxicity	-			

KL = Klimisch criteria

Ref = Reference number

2.5. Data availability matrix

Summary of the available data for all SIDS endpoints.

Hydroxybenzenesulphonic acid CAS 1333-39-7				
	Value	Comment/Species	KL	Ref
Physicochemical properties				
Melting point (°C)	129	calculated	2	3
Boiling point (°C)	270	MSDS	4	1,2
Density (g/cm ³)	1.35	MSDS	4	1,2
Vapor pressure (hPa)	4.4E-07	calculated	2	3
Partition coefficient (log K _{ow})	-1.65	calculated	2	3
	100 vol%		4	1,2
Water solubility (mg/L)	1000	calculated	2	3
Dissociation constant (pKa)	-2.19/9.05		2	4
Environmental fate				
Photodegradation (t _{1/2})	17.3 hours		2	3
Hydrolysis (t _{1/2})	-			
Distribution in water/air/soil/sediment	99.8/0.0/0.0/0.17 %	calculated (emission to water only)	2	3
Ready biodegradability	-			
Ecotoxicity				
Acute fish (96-h LC50, mg/L)	45329	calculated	4	3
Acute invertebrates (96-h EC50, mg/L)	2916	calculated	4	3
Algal inhibition (EC50, mg/L)	1.5E06	calculated	4	3
Mammalian toxicity				
Acute toxicity				
Acute oral (LD50, mg/kg)	1900	rat	4	8,9
	1500	mouse	4	

Hydroxybenzenesulphonic acid CAS 1333-39-7				
	Value	Comment/Species	KL.	Ref
Acute dermal (LD50, mg/kg)	-			
Acute inhalation (LC50, mg/m ³)	-			
Genetic toxicity				
in vitro gene mutation (Ames test)	-			
Chromosomal aberration	-			
Repeated dose	-			
Repro/developmental toxicity	-			

KL. = Klimisch criteria

Ref = Reference number

3. Data availability and testing proposal

The availability of data is depicted in the following table. The study that should be performed to fill a data gap has been indicated.

	Hydroxybenzenesulphonic acid CAS 1333-39-7
Physico-chemical	
Melting point	+
Boiling point	+
Density	+
Vapor Pressure	+
Partition Coefficient	+
Water Solubility	+
Environmental Fate	
Photodegradation	+
Hydrolysis	+
Distribution in compartments	+
Biodegradability	OECD302
Ecotoxicity*	
96-h LC50 Fish	OECD203
48-h EC50 Daphnia	OECD202
72-h EC50 Algal Inhibition	OECD201
Mammalian toxicity	
Acute	+
Repeated dose	OECD422
Genetic Toxicity	OECD471 + OECD 473
Reproduction/developmental	OECD422

* two out of three should be tested

+ = data available

OECD = test to be performed

Adequate physicochemical data are available. For environmental fate only biodegradability has to be tested. For ecotoxicity two of the species have to be investigated. For mammalian toxicity a combined test for repeated dose toxicity and reproduction/developmental toxicity is warranted. Genetic toxicity should be investigated with a standard Ames test and chromosomal aberration study.

4. References

- (1) Dynachem, Inc., MSDS 01/30/95.
- (2) Rütgers Organics Corp., MSDS 12/18/02.
- (3) EPISuite v.3.10, April 2001.
- (4) Pallas 2.1, 1994/95.
- (5) Malaney, GW; McKinney, RE; Oxidative abilities of benzene-acclimated activated sludge; Water Sewage Works 113: 302-9, 1966.
- (6) Alexander, M; Lustigman, BK; Effect of chemical structure on microbial degradation of substituted benzenes; J. Agric. J. Food Chem. 14: 410-3, 1966.
- (7) Kuhn, EP; Suflita, JM; Anaerobic biodegradation of nitrogen-substituted and sulfonated benzene aquifer contaminants; Waste Hazard. Mater. 6 (2): 121-33, 1989.
- (8) SAX's dangerous properties of industrial materials, R.J. Lewis Sr. (Ed.), 9th ed., Van Nostrand Reinhold, NY, 1996.
- (9) Shika Igaku, Odontology 36: 317-322, 1973.

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Appendix

I U C L I D

Data Set

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Existing Chemical : ID: 1333-39-7
CAS No. : 1333-39-7
EINECS Name : hydroxybenzenesulphonic acid
EC No. : 215-587-0
TSCA Name : Benzenesulfonic acid, hydroxy-
Molecular Formula : C6H6O4S

Producer related part
Company : Notox
Creation date : 14.04.2003

Substance related part
Company : Notox
Creation date : 14.04.2003

Status :
Memo :

Printing date : 12.09.2003
Revision date :
Date of last update : 13.08.2003

Number of pages : 14

Chapter (profile) : Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile) : Reliability: without reliability, 1, 2, 3, 4
Flags (profile) : Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE),
Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

2. Physico-Chemical Data

Id 1333-39-7
Date 12.09.2003

2.1 MELTING POINT

Value : = 129 °C
Sublimation :
Method : other: calculated
Year :
GLP :
Test substance :

Test substance : CAS 1333-39-7 (hydroxybenzenesulphonic acid).
Reliability : (2) valid with restrictions
28.04.2003

(1)

2.2 BOILING POINT

Value : = 270 °C at

Remark : Boiling point is 518 °F.
Test substance : CAS 1333-39-7 (hydroxybenzenesulphonic acid), 65% in water.
Reliability : (4) not assignable
22.04.2003

(2) (3)

2.3 DENSITY

Type : relative density
Value : ca. 1.35 at 25 °C

Test substance : CAS 1333-39-7 (hydroxybenzenesulphonic acid), purity not indicated.
Reliability : (4) not assignable
22.04.2003

(3)

Type : relative density
Value : = 1.33 - 1.375 at °C

Test substance : CAS 1333-39-7 (hydroxybenzenesulphonic acid), 65% in water.
Reliability : (4) not assignable
15.04.2003

(2)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value : = .00000044 at 25 °C
Decomposition :
Method : other (calculated)
Year :
GLP :
Test substance :

2. Physico-Chemical Data

Id 1333-39-7
Date 12.09.2003

Test substance : CAS 1333-39-7 (hydroxybenzenesulphonic acid).
Reliability : (2) valid with restrictions
28.04.2003

(1)

2.5 PARTITION COEFFICIENT

Partition coefficient : octanol-water
Log pow : = -1.65 at °C
pH value :
Method : other (calculated)
Year :
GLP :
Test substance :

Test substance : CAS 1333-39-7 (hydroxybenzenesulphonic acid).
Reliability : (2) valid with restrictions
15.04.2003

(1)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Value : = 1000 g/l at 25 °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :

Test substance : CAS 1333-39-7 (hydroxybenzenesulphonic acid).
Reliability : (2) valid with restrictions
15.04.2003

(1)

Solubility in : Water
Value : 100 vol% at 25 °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :

Test substance : CAS 1333-39-7 (hydroxybenzenesulphonic acid), 65% in water.
Reliability : (4) not assignable
22.04.2003

(2) (3)

2.6.2 SURFACE TENSION

2. Physico-Chemical Data

Id 1333-39-7
Date 12.09.2003

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

Memo : pKa calculated

Remark : The pKa was calculated to be -2.19 for the sulphonate group and 9.05 for the hydroxyl group.

Reliability : (2) valid with restrictions
15.04.2003

(4)

3. Environmental Fate and Pathways

Id 1333-39-7

Date 12.09.2003

3.1.1 PHOTODEGRADATION

Type : air
Light source :
Light spectrum : nm
Relative Intensity : based on intensity of sunlight

Remark :

AOP Program (v1.90) Results:

=====

SMILES : Oc1ccc(cc1)S(=O)(=O)O

CHEM :

MOL FOR: C6 H6 O4 S1

MOL WT : 174.17

----- SUMMARY (AOP v1.90): HYDROXYL RADICALS -----

Hydrogen Abstraction = 0.0000 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.2800 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
**Addition to Aromatic Rings = 7.1252 E-12 cm3/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 7.4052 E-12 cm3/molecule-sec

HALF-LIFE = 1.444 Days (12-hr day; 1.5E6 OH/cm3)

HALF-LIFE = 17.333 Hrs

..... ** Designates Estimation(s) Using ASSUMED Value(s)

----- SUMMARY (AOP v1.90): OZONE REACTION -----

***** NO OZONE REACTION ESTIMATION *****
(ONLY Olefins and Acetylenes are Estimated)

Test substance : NOTE: Reaction with Nitrate Radicals May Be Important!
Reliability : CAS 1333-39-7 (hydroxybenzenesulphonic acid).
15.04.2003 : (2) valid with restrictions

(1)

3.1.2 STABILITY IN WATER

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3. Environmental Fate and Pathways

Id 1333-39-7
Date 12.09.2003

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III
Media :
Air : % (Fugacity Model Level I)
Water : % (Fugacity Model Level I)
Soil : % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : % (Fugacity Model Level II/III)
Method : other: calculated
Year :

Remark : Level III Fugacity Model (Full-Output):

=====

Chem Name :
Molecular Wt: 174.17
Henry's LC : 2.62e-013 atm-m3/mole (Henrywin program)
Vapor Press : 3.33e-007 mm Hg (Mpbpwin program)
Liquid VP : 3.54e-006 mm Hg (super-cooled)
Melting Pt : 129 deg C (Mpbpwin program)
Log Kow : -1.65 (Kowwin program)
Soil Koc : 0.00918 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	3.6e-014	34.7	0
Water	99.8	360	1000
Soil	8.73e-008	360	0
Sediment	0.166	1.44e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	1.38e-025	2.47e-012	1.23e-012	2.47e-013	1.23e-013
Water	2.57e-018	658	342	65.8	34.2
Soil	8.32e-026	5.76e-007	0	5.76e-008	0
Sediment	2.14e-018	0.274	0.0114	0.0274	0.00114

Persistence Time: 342 hr
Reaction Time: 520 hr
Advection Time: 1e+003 hr
Percent Reacted: 65.8
Percent Advected: 34.2

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):

Air: 34.66
Water: 360
Soil: 360
Sediment: 1440
Biowin estimate: 3.013 (weeks)

Advection Times (hr):

Air: 100
Water: 1000
Sediment: 5e+004

Test substance : CAS 1333-39-7 (hydroxybenzenesulphonic acid).
Reliability : (2) valid with restrictions

3. Environmental Fate and Pathways

Id 1333-39-7
Date 12.09.2003

13.08.2003

(1)

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : aerobic
Inoculum : activated sludge, adapted
Concentration : 500 mg/l related to Test substance
related to
Contact time : 72 hour(s)
Degradation : (±) % after
Result :
Deg. product :
Method : other: not indicated
Year : 1966
GLP : no
Test substance :

Method : INOCULUM/TEST ORGANISM
- Inoculum: 5000 mg/L in test solution
- Source: sewage treatment plant
- Preparation of inoculum: fill-and-draw unit containing 1.5 L of mixed liquor; air was supplied at a rate to keep the floc in suspension; every 24 hours the air was shut off and the floc allowed to settle; 1 L of supernatant liquor was wasted and was replaced by an equivalent volume of nutrient solution containing glucose (500 mg/L). Then gradually increased amounts of benzene were added over a 20-day period until benzene had reached a concentration of 250 mg/L.
- Pretreatment: benzene-fed (sole source of carbon); the inoculum used is then taken 16 hr after batch feeding and concentrated to 5000 mg/L

TEST SYSTEM

- Preparation of test solution: 10 ml of adapted sludge suspension (5000 mg/L) and 10 ml of test substance solution (1000 mg/L in 2% phosphate buffer (pH 7.0-7.3))
- Initial test substance concentration (mg C/L): 207 mg C/L (500 mg test substance/L)
- Culturing apparatus: Warburg constant-column respirometer with 125-ml flasks
- Number of culture flasks per concentration: not indicated
- Test duration: 72 hours
- Sampling: at about 28, 40, 54 and 72 hours
- Analytical parameter: oxygen consumption
- ThOD: 1.287 mg/mg (= 643.5 mg O₂/L)

TEST CONDITIONS

- Composition of mineral solution: 500 mg/L dibasic potassium phosphate, 500 mg/L Calgonite, 325 mg/L ammonium phosphate and 50 mg/L ferric chloride in tap water
- Test temperature: 20 °C

3. Environmental Fate and Pathways

Id 1333-39-7

Date 12.09.2003

Result : CONTROLS: inoculum only
: The oxygen uptake has been graphically depicted. The oxygen uptake is lower for p-phenolsulphonic acid than for the control. The test substance inhibits the microorganisms in the benzene-adapted sludge.

Test substance : other TS: CAS 98-67-9 (p-hydroxybenzenesulphonic acid), purity analytical grade.

Reliability : (4) not assignable
: 1. The information is limited to the above mentioned.
: 2. The test is no guideline test. Adapted microorganisms are used. The concentration of the test substance and of the inoculum are higher than in OECD 302C (30 mg/L and 100 mg/L for test substance and inoculum is recommended, respectively).

22.04.2003

(5)

Type : aerobic
Inoculum : other: soil microorganisms
Concentration : 75 mg/l related to Test substance related to

Deg. product :
Method : other: not indicated
Year : 1966
GLP : no
Test substance :

Method : INOCULUM/TEST ORGANISM
: - Inoculum: 1.0 ml of 1% suspension of Niagara silt loam

TEST SYSTEM

- Initial test substance concentration: 31 mg C/L
- Culturing apparatus: 45 mm diameter X 80 mm high screw-cap bottles containing 40 ml of medium
- Number of culture flasks per concentration: 2 for test substance + inoculum; 2 for test substance + inoculum + HgCl₂ (abiotic control); 2 for 1% glucose controls
- Measuring equipment: Beckman spectrophotometer
- Test duration: 64 days
- Sampling: samples were taken after mixing, at intervals of 3 to 6 hours and at 1, 2, 4, 8, 16, 32 and 64 days after inoculation
- Analytical parameter: absorbance at 260 nm relative to soil-medium mixture without chemical

TEST CONDITIONS

- Composition of mineral solution: 1.6 g K₂HPO₄, 0.40 g KH₂PO₄, 0.50 g NH₄NO₃, 0.20 g MgSO₄·7H₂O, 25 mg CaCl₂·2H₂O, 2.3 mg FeCl₃·6H₂O in 1 L of distilled water
- Test temperature: 25 °C

Result : The time necessary for complete degradation was established to be 32 days. The degradation was due to biological activity, because no decreased absorbance was seen in vessels with HgCl₂.

Test substance : other TS: CAS 98-67-9 (p-hydroxybenzenesulphonic acid), purity not indicated.

Reliability : (4) not assignable
: The information was limited to the above mentioned.

28.04.2003

(6)

Type : anaerobic

3. Environmental Fate and Pathways

Id 1333-39-7

Date 12.09.2003

Inoculum : other: aquifer microorganisms
Concentration : .2 mmol/l related to Test substance
related to
Contact time : 13 month
Degradation : (±) % after
Result :
Deg. product :
Method : other: not indicated
Year : 1989
GLP : no data
Test substance :

Remark : The test substance was inoculated with aquifer slurry from two sites near a municipal landfill: a methanogenic site (TOC 288 mg/L and sulfate concentration < 0.1 mM) and a sulfate reducing site (TOC 14.4 mg/L and sulfate concentration 2.1 mM). Experiments were performed in the dark at room temperature in duplicate with sterilised aquifer slurries as control. Disappearance of the test substance was analysed by reversed-phase HPLC with UV detection at 275 nm.
Results:
Sulphate-reducing slurry (0, 13 months): 188, 198 µM
Methanogenic slurry (0, 13 months): 194, 235 µM
Test substance : other TS: CAS 98-67-9 (p-hydroxybenzenesulphonic acid), purity not indicated.
Conclusion : No biodegradation was observed for p-hydroxybenzenesulphonic acid.
Reliability : (4) not assignable
22.04.2003 (7)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4. Ecotoxicity

Id 1333-39-7
Date 12.09.2003

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type :
Species :
Exposure period : 96 hour(s)
Unit : mg/l
LC50 : = 45329
Method : other: calculated
Year :
GLP :
Test substance :

Remark : Value calculated for ECOSAR class phenol-acid.
Test substance : CAS 1333-39-7 (hydroxybenzenesulphonic acid).
Reliability : (4) not assignable
28.04.2003

(1)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type :
Species : Daphnia magna (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
EC50 : = 2916
Method : other: calculated
Year :
GLP :
Test substance :

Remark : Value calculated for ECOSAR class phenol-acid.
Test substance : CAS 1333-39-7 (hydroxybenzenesulphonic acid).
Reliability : (4) not assignable
28.04.2003

(1)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species : other algae: green algae
Endpoint :
Exposure period : 96 hour(s)
Unit : g/l
EC50 : = 1500
Method : other: calculated
Year :
GLP :
Test substance :

Remark : Value calculated for ECOSAR class phenol-acid.
Test substance : CAS 1333-39-7 (hydroxybenzenesulphonic acid).
Reliability : (4) not assignable
28.04.2003

(1)

4. Ecotoxicity

Id 1333-39-7
Date 12.09.2003

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5. Toxicity

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Date 12.09.2003

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type : LD50
Value : = 1900 mg/kg bw
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Method :
Year : 1973
GLP :
Test substance :

Remark : Mean value of males and females.
Test substance : CAS 1333-39-7 (hydroxybenzenesulphonic acid), purity not indicated.
Reliability : (4) not assignable
03.06.2003 (8) (9)

Type : LD50
Value : = 1500 mg/kg bw
Species : mouse
Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Method :
Year : 1973
GLP :
Test substance :

Remark : Mean value of males and females is 1525 mg/kg.
Test substance : CAS 1333-39-7 (hydroxybenzenesulphonic acid), purity not indicated.
Reliability : (4) not assignable
03.06.2003 (8) (9)

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5. Toxicity

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5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

9. References

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Date 12.09.2003

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